THE SHORT-RANGE EXPANSION IN SOLID STATE

Helge Holden

Raphael Høegh-Krohn

Steinar Johannesen

Matematisk institutt
Universitetet i Oslo
Blindern, Oslo 3
Norge

Abstract:

We study the universal behaviour of the one-electron approximation in solid state with a short- and zero-range interaction in three dimensions. More precisely, let $H_\varepsilon = -\Delta+\varepsilon^{-2}\mu(\varepsilon) \sum_{\lambda\in\Lambda} V(\frac{1}{\varepsilon}(\cdot-\lambda))$ where V is a short-range potential, μ analytic with $\mu(0) = 1$ and Λ is a lattice modelling an infinite crystal, an infinite straight polymer or an infinite monomolecular layer. We show that H_ε converges in norm resolvent sense to the Hamiltonian with point interactions. Decomposing $H_\varepsilon = \int_{\hat{\Lambda}}^{\oplus} H_\varepsilon(\theta)d\theta$ where $\hat{\Lambda}$ is the Brillouin zone (the dual of Λ) we expand the eigenvalues and resonances of $H_\varepsilon(\theta)$ explicitly to first order in ε. The first order term has a simple form.

1. Introduction.

The well-known Kronig-Penney model [9] provides an explicitly solvable model of an infinite crystal in one dimension. The model is simply the one electron approximation with a δ-potential interaction.

It was recently discovered by Grossmann, Høegh-Krohn and Mebkhout [4] that it is also possible to give a rigorous definition of an analogue of the Kronig-Penney model in three dimensions. But the definition is much more subtle than in one dimension and it is necessary with a renormalization procedure. However, the model is still solvable and the spectral properties of it has been thoroughly studied by Grossmann, Høegh-Krohn and Mebkhout [5] and Høegh-Krohn, Holden, Martinelli [6].

In this paper we study in which sense this solvable model with zero-range interactions is well approximated by more realistic short-range interactions.

More precisely, let the Hamiltonian H be given by

$$H_\varepsilon = -\Delta+\varepsilon^{-2}\sum_{j=1}^{\infty}\mu_j(\varepsilon)V_j(\tfrac{1}{\varepsilon}(\cdot-x_j)) \qquad (1.1)$$

where the V_j's are suitable short-range potentials, e.g. compact support and the μ_j's are real-valued analytic functions with $\mu(o) = 1$.

We note that $\varepsilon^{-3}V(\frac{1}{\varepsilon}(x-x_j)) \to \delta(x-x_j)$ as $\varepsilon \to 0$, while we have $\varepsilon^{-2}V(\frac{1}{\varepsilon}(x-x_j)) = \varepsilon(\varepsilon^{-3}V(\frac{1}{\varepsilon}(x-x_j)))$ which indicates that the limit $\varepsilon \to 0$ is not a trivial object to study and that some renormalization procedure is necessary to define point interactions rigorously.

In this paper we prove that H_ε tends to the point interaction Hamiltonian as ε tends to zero in norm resolvent sense. This extends a result by Albeverio and Høegh-Krohn [3] where convergence in strong resolvent sense is proved, and where also the case with only a finite number of terms in the sum is discussed. Stronger results in this latter case where however obtained by Albeverio, Gesztesy and Høegh-Krohn [1] and Holden, Høegh-Krohn and Johannesen [7].

The result is applied to the situation where the set $\{x_j\}$ forms a lattice Λ and $V_j \equiv V$, $\mu_j \equiv \mu$. This makes the Hamiltonian H_ε translation invariant under Λ and we can decompose the Hamiltonian as

$$H_\varepsilon = \int_{\hat{\Lambda}}^{\oplus} H_\varepsilon(\theta)d\theta \tag{1.2}$$

where $\hat{\Lambda} \equiv \underline{\underline{R}}^3/\Gamma$ and Γ is the orthogonal lattice to Λ (for more datails see section 3, 4 and 5). The negative part of the spectrum of $H_\varepsilon(\theta)$ consists of discrete eigenvalues and we obtain analytic expansion around the point interaction eigenvalue. The surprising fact is that if $E_0(\theta)$ denotes the eigenvalue of the decomposed point interaction operator and $E_\varepsilon(\theta)$ is an eigenvalue for $H_\varepsilon(\theta)$ converging to $E_0(\theta)$ we have the expansion

$$E_\varepsilon(\theta) = E_0(\theta)+\varepsilon E_1(\theta)+o(\varepsilon) \tag{1.3}$$

where

$$E_1(\theta) = h_\Lambda^\theta(A+E_0(\theta)B) \tag{1.4}$$

and h_Λ^θ depends only on the lattice and θ. A,B are independent of the lattice and θ and only depend on properties of the one-center operator $-\Delta+V$. For the explicit form of h_Λ^θ and A and B see the next sections. The expansion also applies to the positive part of the spectrum and is independent of whether the lattice Λ is 1-, 2- or 3-dimensional.

The point interaction model of a straight polymer, i.e. when Λ is 1-dimensional, exhibits real resonances and also in this case the expansion (1.3) is valid. We note the resonances are still real to first order in ε.

2. Approximation to point interactions.

We consider a countable subset $X = \{x_j\}$ of $\mathbb{R}^3$ which is discrete in the sense that $\inf_{i \neq j} |x_i - x_j| > 0$ and a countable set of potentials $\{V_j\}$ such that:

There exists a real Rollnik function V (i.e. $V: \mathbb{R}^3 \to \mathbb{R}$ and $\iint |V(x)||V(y)||x-y|^{-2} dx dy < \infty$) with compact support such that

$$|V_j| \leq V \tag{2.1}$$

for all j.

See Simon [13] for properties of Rollnik functions. Let $\{\mu_i\}$ be a countable set of real analytic functions uniformly bounded in a neighbourhood of 0 with $\mu_j(0) = 1$ for all j. By Δ we denote the self-adjoint Laplacian on $L^2(\mathbb{R}^3)$. With these definition we have the following.

Lemma 2.1. The Hamiltonian

$$H_\varepsilon = -\Delta + \varepsilon^{-2} \sum_{j=1}^{\infty} \mu_j(\varepsilon) V_j\left(\frac{1}{\varepsilon}(\cdot - x_j)\right) \tag{2.2}$$

is a self-adjoint operator on $L^2(\mathbb{R}^3)$ defined in terms of quadratic forms for small $\varepsilon > 0$.

Proof: Let

$$W(x) = \varepsilon^{-2} \sum_{j=1}^{\infty} \mu_j(\varepsilon) V_j\left(\frac{1}{\varepsilon}(x - x_j)\right) \tag{2.3}$$

for ε so small that $\operatorname{supp} V_i\left(\frac{1}{\varepsilon}(\cdot - x_i)\right) \cap \operatorname{supp} V_j\left(\frac{1}{\varepsilon}(\cdot - x_j)\right) = \emptyset$ for all $i \neq j$. By the KLMN theorem (see Reed-Simon II [10]) it is enough to prove that $W \lll -\Delta$.

Let G_E now denote the resolvent of the free Hamiltonian, i.e.

$$G_E = (-\Delta - E)^{-1} \tag{2.4}$$

In $L^2(\underline{\underline{R}}^3)$ G_E has an integralkernel which we denote by $G_E(x-y)$ which is given by

$$G_E(x-y) = \frac{e^{i\sqrt{E}|x-y|}}{4\pi|x-y|} \tag{2.5}$$

where $\operatorname{Im}\sqrt{E} > 0$.

As in the proof of theorem 1.21 in Simon [13] we only need to prove that given $a > 0$ there exists an E such that

$$\langle \phi, |W|^{\frac{1}{2}} G_E |W|^{\frac{1}{2}} \phi \rangle \leqslant a^2 \|\phi\|^2 \tag{2.6}$$

for all $\phi \in C_0^\infty(\underline{\underline{R}}^3)$.

Let

$$w_j(x) = \varepsilon^{-1} |\mu_j(\varepsilon) V_j(\tfrac{1}{\varepsilon}(x-x_j))|^{\frac{1}{2}} \tag{2.7}$$

and let χ_j be the characteristic function for $\operatorname{supp} w_j$ and define $\chi_0 = 1 - \sum_{j=1}^\infty \chi_j$ and $\phi_j = \chi_j \phi$.

Then

$$\begin{aligned}
&\langle \phi, |W|^{\frac{1}{2}} G_E |W|^{\frac{1}{2}} \phi \rangle \\
&= \sum_{j=1}^\infty \langle \phi_j, \sum_{\ell=1}^\infty w_j G_E w_\ell \phi_\ell \rangle \\
&\leqslant \|\phi\| \Big(\sum_{j=1}^\infty \| \sum_{\ell=1}^\infty w_j G_E w_\ell \phi_\ell \| \Big)^{\frac{1}{2}} \\
&\leqslant \|\phi\|^2 \| [w_j G_E w_\ell]_{j,\ell=1}^\infty \|_H
\end{aligned} \tag{2.8}$$

from the appendix where $\| \ \|_H$ denotes the Holmgren norm (see appendix). From the explicit expression for the kernel of the resolvent G_E we see that $\|[w_j G_E w_\ell]\|_H$ can be made arbitrarily small by choosing E such that $\operatorname{Im}\sqrt{E}$ is large.

Let now

$$v_j = |V_j|^{\frac{1}{2}} \quad \text{and} \quad u_j = v_j \operatorname{sgn} V_j \tag{2.9}$$

where sgn denotes the signum function, $\operatorname{sgn}(x) = \begin{cases} 1 & x > 0 \\ 0 & x = 0. \\ -1 & x < 0 \end{cases}$

We introduce the Hilbert space

$$\mathcal{H} = \bigoplus_{j=1}^{\infty} L^2(\underline{\underline{R}}^3) \tag{2.10}$$

and the operators

$$\begin{aligned} D^{\varepsilon} &: L^2(\underline{\underline{R}}^3) \to \mathcal{H} \\ B^{\varepsilon} &: \mathcal{H} \to \mathcal{H} \\ C^{\varepsilon} &: \mathcal{H} \to L^2(\underline{\underline{R}}^3) \end{aligned} \tag{2.11}$$

with integral kernels

$$\begin{aligned} D_j^{\varepsilon}(x,y) &= \mu_j(\varepsilon) u_j(x) G_E(\varepsilon x + x_j - y) \\ B_{j\ell}^{\varepsilon}(x,y) &= \varepsilon \mu_j(\varepsilon) u_j(x) G_E(\varepsilon(x-y) + x_j - x_\ell) v_\ell(y) \\ C_j^{\varepsilon}(x,y) &= G_E(x - \varepsilon y - x_j) v_j(y). \end{aligned} \tag{2.12}$$

(We suppress the E dependence for the moment in the notation.)

For these operators we have

<u>Lemma 2.2</u>. B^{ε}, C^{ε} and D^{ε} are bounded operators and $\|B^{\varepsilon}\|$ can be made arbitrarily small when $\operatorname{Im}\sqrt{E}$ is chosen sufficiently large.

<u>Proof</u>: We have

$$\begin{aligned} &\sup_{\ell} \sum_{j=1}^{\infty} \|B_{\ell j}^{\varepsilon}\| \le \\ &\sup_{\ell} \sum_{j} \varepsilon |\mu_j(\varepsilon)| \left[\iint \frac{|V_\ell(x)|\,|V_j(y)|}{(4\pi)^2 |\varepsilon(x-y)+x_\ell-x_j|^2} e^{-2\operatorname{Im}\sqrt{E}|\varepsilon(x-y)+x_\ell-x_j|} dxdy \right]^{\frac{1}{2}} \end{aligned} \tag{2.13}$$

which can be made arbitrarily small when $\mathrm{Im}\sqrt{E}$ is sufficiently large, and similar for $\sup_j \sum_{\ell=1}^{\infty} \|B^{\varepsilon}_{\lambda j}\|$. This implies that also $\|B^{\varepsilon}\|_H$ can be made arbitrarily small. For $\psi \in L^2(\underline{\underline{R}}^3)$ we have:

$$\sum_j \|D^{\varepsilon}_j \psi\|^2 = \sum_j \mu_j(\varepsilon)^2 \int |V_j(x)| \, |\int \frac{e^{i\sqrt{E}|\varepsilon x+x_j-y|}}{4\pi|\varepsilon x-x_j-y|} \psi(y)dy|^2 dx \tag{2.14}$$

$$\leq \sum_j \mu_j(\varepsilon)^2 \int |V_j(x)|dx \int \frac{e^{-\mathrm{Im}\sqrt{E}|\varepsilon x+x_j-y|}}{(4\pi)^2|\varepsilon x+x_j-y|^2} dy \int e^{-\mathrm{Im}\sqrt{E}|\varepsilon x+x_j-y|} |\psi(y)|^2 dy$$

$$\leq \sup_j \mu_j(\varepsilon)^2 \int \frac{e^{-\mathrm{Im}\sqrt{E}|y|}}{(4\pi)^2|y|^2} dy \int |V(x)|dx \int \sum_j e^{-\mathrm{Im}\sqrt{E}|\varepsilon x+x_j-y|} |\psi(y)|^2 dy$$

$$\leq c\|V\|_1 \|\psi\|_2^2$$

where c is a constant, showing that D^{ε} is bounded. A similar argument shows that $(C^{\varepsilon})^*$ is bounded, thus making C^{ε} bounded.

We can now state the following theorem which was first proved for a finite number of centers (i.e. with $H = \bigoplus_{i=1}^{N} L^2(\underline{\underline{R}}^3)$ with $N < \infty$) in Holden, Høegh-Krohn and Johannesen [7]. See also Albeverio et al [2] for an abstract version of the finite center case.

<u>Theorem 2.3.</u> When $E \notin \sigma(H_{\varepsilon})$

$$(H_{\varepsilon}-E)^{-1} = G_E - \varepsilon C^{\varepsilon}(1+B^{\varepsilon})^{-1}D^{\varepsilon} \tag{2.15}$$

<u>Proof:</u> The proof is in 3 steps.

<u>Step 1:</u>
$$(G_E \sum_{j=1}^{\infty} W_j)^m G_E = \varepsilon C^{\varepsilon}(B^{\varepsilon})^{m-1}D^{\varepsilon} \tag{2.16}$$

where $W_j(x) = \varepsilon^{-2}\mu_j(\varepsilon)V_j(\frac{1}{\varepsilon}(x-x_j))$ and $m \in \underline{\underline{N}}$.

<u>Proof:</u> We define the functions:

$$\begin{aligned} \tilde{u}_j(x) &= u_j(\tfrac{1}{\varepsilon}(x-x_j)) \\ \tilde{v}_j(x) &= v_j(\tfrac{1}{\varepsilon}(x-x_j)) \\ \tilde{w}_j(x) &= \varepsilon^{-2}\mu_j(\varepsilon)\tilde{u}_j(x). \end{aligned} \tag{2.17}$$

Let $A: \mathcal{H} \to \mathcal{H}$ be the operator with components $A_{j\ell} = \tilde{w}_j G_E \tilde{v}_\ell$. Then:

$$(2.18)\quad \begin{aligned}(G_E \sum_{j=1}^{\infty} W_j)^m G_E &= (G_E \sum_{j=1}^{\infty} \tilde{v}_j \tilde{w}_j)^m G_E \\ &= \sum_{j_1,\dots,j_m} G_E \tilde{v}_{j_1} A_{j_1 j_2} \cdots A_{j_{m-1} j_m} \tilde{w}_{j_m} G_E \\ &= \sum_{j_1,\dots,j_m} \varepsilon C^{\varepsilon}_{j_1} B^{\varepsilon}_{j_1 j_2} \cdots B^{\varepsilon}_{j_{m-1} j_m} D^{\varepsilon}_{j_m} = \varepsilon C^{\varepsilon}(B^{\varepsilon})^{m-1} D^{\varepsilon}\end{aligned}$$

using a change in variables.

<u>Step 2</u>: $(H_\varepsilon - E)^{-1} = G_E + \sum_{m=1}^{\infty} (-1)^m [G_E \sum_{j=1}^{\infty} W_j]^m G_E$ (2.19)

for $\mathrm{Im}\sqrt{E}$ large.

<u>Proof</u>: Using step 1 and lemma 2.2 we see that the right hand side of (2.19) is norm convergent when $\mathrm{Im}\sqrt{E}$ is large. The formula then follows as in lemma II.11 in Simon [13].

<u>Step 3</u>: Combining now step 1 and 2 we have

$$(2.20)\quad \begin{aligned}(H_\varepsilon - E)^{-1} &= G_E + \varepsilon \sum_{m=1}^{\infty} (-1)^m C^{\varepsilon}(B^{\varepsilon})^{m-1} D^{\varepsilon} \\ &= G_E - \varepsilon C^{\varepsilon}(1+B^{\varepsilon})^{-1} D^{\varepsilon} \quad \text{when } \mathrm{Im}\sqrt{E} \text{ is large.}\end{aligned}$$

The theorem follows by analytic continuation on both sides.

We now assume in addition that

(i) 0 is a simple zero energy resonance for $-\Delta + V_j$ for $j \in N$, i.e. -1 is a simple eigenvalue for $u_j G_0 v_j$ with eigenfunction ϕ_j such that $\phi_j = G_0 v_j \phi_j$, which fullfils $(-\Delta + V_j)\phi_j = 0$ in the sense of distributions, is <u>not</u> in $L^2(\underline{\underline{R}}^3)$. For later use we define $\tilde{\phi}_j = \phi_j \operatorname{sgn} V_j$ which fullfils $(1 + v_j G_0 u_j)\tilde{\phi}_j = 0$. A very convenient criterium to decide when ϕ is in $L^2(\underline{\underline{R}}^3)$

is the following. We have that $\phi_j \in L^2\underline{\underline{R}}^3)$ iff $(v,\phi_j) = 0$. (See Albeverio, Gesztesy, Høegh-Krohn [1].)

(ii) There exists an interval I around 1 such that $-\Delta+\lambda V_j$ has no zero energy resonances for $\lambda \in I \setminus \{1\}$ when $j \in \underline{\underline{N}}$.

<u>Remark</u>: For a discussion of assumption (i) in the finite center case, see Albeverio, Høegh-Krohn [3], Albeverio, Gesztesy, Høegh-Krohn [1] and Holden, Høegh-Krohn, Johannesen [7].

We will now introduce the Hamiltonian corresponding to the formal operator

$$-\Delta_X = -\Delta - \sum_{j=1}^{\infty} \nu_j \delta(\cdot - x_j) \tag{2.21}$$

where $X = (x_1,\ldots,x_n,\ldots)$, $\nu = (\nu_1,\ldots,\nu_n,\ldots)$ with $\nu_j \in \underline{\underline{R}}$ and δ is Dirac's delta function.

This formal operator can be rigorously defined as the unique self-adjoint operator $-\Delta_{(X,\alpha)}$ on $L^2(\underline{\underline{R}}^3)$ with resolvent which has an integralkernel defined by:

$$(-\Delta_{(X,\alpha)}-E)^{-1}(x,y) = \tag{2.22}$$

$$G_E(x-y)+\sum_{j,\ell=1}^{\infty} [(\alpha_j - \frac{i\sqrt{E}}{4\pi})\delta_{j\ell} - \tilde{G}_E(x_j-x_\ell)]^{-1}_{j\ell} G_E(x-x_j)G_E(x_\ell-y)$$

where $\operatorname{Im}\sqrt{E} > 0$,

$$\tilde{G}_E(x) = \begin{cases} G_E(x) & x \neq 0 \\ 0 & x = 0 \end{cases} \tag{2.23}$$

$\alpha = (\alpha_1,\ldots,\alpha_n,\ldots)$, $\alpha_n \in \underline{\underline{R}}^3$, and $[\ ]^{-1}$ is the inverse of the matrix $[\ ]$ on $l^2(X)$. See Grossmann, Høegh-Krohn and Mebkhout [4], [5] for this definition and the relation between the ν_j of (2.21) and the α_j of (2.22). Using this definition we can state the main theorem in this section.

Theorem 2.4. Under the general assumptions stated in the beginning of this section and assumptions (i) and (ii) we have that H_ε converges to $-\Delta_{(X,\alpha)}$ in norm resolvent sense as $\varepsilon \to 0$ where $\alpha = (\alpha_1,\ldots,\alpha_n,\ldots)$ has components

$$\alpha_j = \mu_j'(0)(\tilde{\phi}_j,\phi_j)|(v_j,\phi_j)|^{-2}. \tag{2.24}$$

Remarks:

1. In Albeverio, Høegh-Krohn [3] it is proved strong convergence in the resolvent sense.
2. In the one-dimensional case (i.e. as operators on $L^2(\underline{R})$) this is proved in Albeverio et al [2]. However, in one dimension both $-\Delta_{(X,\alpha)}$ and $G_E(x)$ are given by other expressions than in three dimensions.
3. In the finite center case this is proved in Holden, Høegh Krohn and Johannesen [7] and in the one-center case in Albeverio, Gesztesy and Høegh-Krohn [1].

Proof: Using theorem 2.3 we only have to find the limit of the operators $(1+B^\varepsilon)^{-1}$, C^ε, D^ε as ε tends to zero.

When $\psi \in L^2(\underline{\underline{R}}^3)$ we have (for simplicity we assume $\mu_j \equiv 1$)

$$\sum_{j=1}^\infty \|(D_j^\varepsilon - D_j^0)\psi\|^2$$

$$= \sum_{j=1}^\infty \int |v_j(x)|\,|\int[\frac{e^{i\sqrt{E}|\varepsilon x+x_j-y|}}{4\pi|\varepsilon x+x_j-y|} - \frac{e^{i\sqrt{E}|x_j-y|}}{4\pi|x_j-y|}]\psi(y)dy|^2 dx$$

$$\leqslant \sum_{j=1}^\infty \int |v_j(x)|\int|\frac{e^{i\sqrt{E}|\varepsilon x+x_j-y|}}{4\pi|\varepsilon x-x_j-y|} - \frac{e^{i\sqrt{E}|x_j-y|}}{4\pi|x_j-y|}|^2 e^{2\mathrm{Im}\sqrt{E}|x_j-y|}dy$$

$$\cdot \int e^{-2\mathrm{Im}\sqrt{E}|x_j-y|}|\psi(y)|^2 dydx \tag{2.25}$$

$$\leqslant \int|V(x)|\int|\frac{e^{i\sqrt{E}|\varepsilon x+y|}}{4\pi|\varepsilon x+y|} - \frac{e^{i\sqrt{E}|y|}}{4\pi|y|}|^2 e^{2\mathrm{Im}\sqrt{E}|y|}dy$$

$$\cdot \int\sum_j e^{-2\mathrm{Im}\sqrt{E}|x_j-y|}|\psi(y)|^2 dydx$$

$$= c(\varepsilon) \quad \|\psi\|_2^2 \quad \text{where} \quad c(\varepsilon) \to 0 \quad \text{as} \quad \varepsilon \to 0.$$

A similar argument shows that $(C^\varepsilon)^* \overset{n}{\to} (C^0)^*$ and therefore

$$C^\varepsilon \overset{n}{\to} C^0. \tag{2.26}$$

To study $(1+B^\varepsilon)^{-1}$ we split B^ε into the diagonal and off-diagonal elements with kernels:

$$E^\varepsilon_{j\ell}(x,y) = \delta_{j\ell}\mu_j(\varepsilon)u_j(x)G_{\varepsilon^2 E}(x-y)v_j(y) \tag{2.27}$$

$$F^\varepsilon_{j\ell}(x,y) = (1-\delta_{j\ell})\mu_j(\varepsilon)u_j(x)G_E(\varepsilon(x-y)+x_j-x_\ell)v_\ell(y)$$

thus making $1+B^\varepsilon = 1+E^\varepsilon+\varepsilon F^\varepsilon$ and

$$(1+B^\varepsilon)^{-1} = (1+\varepsilon(1+E^\varepsilon)^{-1}F_\varepsilon)^{-1}\,\varepsilon(1+E^\varepsilon)^{-1}. \tag{2.28}$$

We have that $\|F^\varepsilon-F^0\|_H^2 \to 0$ since

$$\sup_j \sum_{\substack{\ell=1\\ \ell\neq j}}^{\infty} \int |V_j(x)|\,\left|\frac{e^{i\sqrt{E}|\varepsilon(x-y)+x_j-x_\ell|}}{4\pi|\varepsilon(x-y)+x_j-x_\ell|} - \frac{e^{i\sqrt{E}|x_j-x_\ell|}}{4\pi|x_j-x_\ell|}\right|^2 |V_\ell(y)|\,dxdy \to 0 \tag{2.29}$$

by dominated convergence theorem.

Expanding E^ε_{jj} in ε we have

$$\mu_j(\varepsilon)u_jG_{\varepsilon^2 E}v_j = u_jG_0v_j+\varepsilon L_j+o_j(\varepsilon) \tag{2.30}$$

where

$$L_j = \mu_j'(0)u_jG_0v_j+\frac{i\sqrt{E}}{4\pi}|u_j\rangle\langle v_j| \tag{2.31}$$

and $\frac{1}{\varepsilon}o_j(\varepsilon) \overset{n}{\to} 0$ as $\varepsilon \to 0$ uniformly in j. (The operator $S = |f\rangle\langle g|$ is defined to be $Sh = f(g,h)$.) In lemma 2.6, proved after this theorem, we show that

$$\varepsilon(1+\varepsilon+u_jG_0v_j)^{-1} = P_j+o_j(1) \tag{2.32}$$

where $P_j = \frac{|\phi_j><\tilde{\phi}_j|}{(\tilde{\phi}_j, \phi_j)}$ is uniformly bounded and $o_j(1) \to 0$ uniformly in j.

From (2.30) and (2.32) we obtain after a short computation (see Holden, Høegh-Krohn and Johannesen [7])

$$\varepsilon(1+E^{\varepsilon})^{-1} = K+o(1) \tag{2.33}$$

where $o(1) \to 0$ as $\varepsilon \to 0$ and

$$K = [\delta_{j\ell}(\frac{i\sqrt{E}}{4\pi}|(v_j,\phi_j)|^2 - \mu_j'(o)(\tilde{\phi}_j,\phi_j))^{-1}|\phi_j><\tilde{\phi}_j|]. \tag{2.34}$$

Using now (2.25), (2.26) and (2.33) we finally obtain

$$(H_{\varepsilon}-E)^{-1} \overset{n}{\to} (-\Delta_{X,\alpha})-E)^{-1} \quad \text{as} \quad \varepsilon \to 0 \tag{2.35}$$

after a computation where α is as defined in the theorem. Before we prove the remaining lemma we state a corrolary.

<u>Corollary 2.5</u>. If there is only a finite number of different potentials we still have that

$$(H_{\varepsilon}-E)^{-1} \overset{n}{\to} (-\Delta_{(X,\alpha)}-E)^{-1} \quad \text{as} \quad \varepsilon \to 0 \tag{2.36}$$

without assumption (ii).

<u>Proof</u>: The only place where we use assumption (ii) is in order to have uniformity in equation (2.32).

<u>Lemma 2.6</u>. With the same assumptions as in theorem 2.4 we have

$$\varepsilon(1+\varepsilon+u_jG_0v_j)^{-1} = P_j+o_j(1) \tag{2.37}$$

where $P_j = \frac{|\phi_j><\tilde{\phi}_j|}{(\tilde{\phi}_j, \phi_j)}$ is bounded uniformly in j and $\|o_j(1)\| \to 0$ uniformly in j.

<u>Proof</u>: From lemma 3.1 in Albeverio, Gesztesy and Høegh Krohn [1] we have the norm convergent expansion

$$\varepsilon(1+\varepsilon+u_jG_0v_j)^{-1} = P_j - \sum_{m=1}^{\infty} \varepsilon^m T_j^m \tag{2.38}$$

where

$$P_j = (2\pi i)^{-1} \oint_{\Gamma_j} dz(z-u_jG_0v_j)^{-1} = \frac{|\phi_j\rangle\langle\tilde{\phi}_j|}{(\phi_j,\tilde{\phi}_j)} \tag{2.39}$$

and

$$T_j = (2\pi i)^{-1} \oint_{\Gamma_j} dz(z+1)^{-1}(z-u_jG_0v_j)^{-1} \tag{2.40}$$

where Γ_j surrounds only the isolated eigenvalue -1 of $u_jG_0v_j$.

We now have that

$$(z-u_jG_0v_j)^{-1} = z^{-1}+z^{-1}u_jG_0^{\frac{1}{2}}(z-G_0^{\frac{1}{2}}V_jG_0^{\frac{1}{2}})^{-1}G_0^{\frac{1}{2}}v_j \tag{2.41}$$

when $z \neq 0$ where $G_0^{\frac{1}{2}}V_jG_0^{\frac{1}{2}}$ is a self-adjoint Hilbert-Schmidt operator. The operator $u_jG_0^{\frac{1}{2}}$ is bounded with:

$$\begin{aligned} \|u_jG_0^{\frac{1}{2}}\|^2 &= \|u_jG^{\frac{1}{2}}(u_jG_0^{\frac{1}{2}})^*\| = \|u_jG_0u_j\| \\ &\leqslant \|u_jG_0u_j\|_2 = \|V_j\|_R \leqslant \|V\|_R \end{aligned} \tag{2.42}$$

where $\|V\|_R = [\iint|V(x)V(y)|\,|x-y|^{-2}dxdy]^{\frac{1}{2}}$ is the Rollnik-norm).

Similarly $\|G_0^{\frac{1}{2}}v_j\|^2 \leqslant \|V\|_R$. Since $G_0^{\frac{1}{2}}VG_0^{\frac{1}{2}}$ is self-adjoint,

$$\|(z-G_0^{\frac{1}{2}}VG_0^{\frac{1}{2}})^{-1}\| = d(z,\sigma(G_0^{\frac{1}{2}}VG_0^{\frac{1}{2}}))^{-1} \tag{2.43}$$

where $d(\cdot,\cdot)$ denotes the distance.

From assumtion (ii) on the potentials there is a neighbourhood U around -1 such that $\sigma(u_jG_0v_j) \cap U = \{-1\}$ for all j.

Since $\sigma(G_0^{\frac{1}{2}}V_jG_0^{\frac{1}{2}}) \cup \{0\} = \sigma(u_jG_0v_j) \cup \{0\}$ there exists a constant c such that

$$d(z, \sigma(G_0^{\frac{1}{2}} V_j G_0^{\frac{1}{2}})) \leq c \qquad (2.44)$$

for all j.

From (2.41) we have that $(z-u_j G_0 v_j)^{-1}$ is uniformly bounded which makes P_j and T_j uniformly bounded.

3. Crystals.

In this section we use the results of section 2 in the case where the set X of points with point interaction forms a lattice, thus modelling an infinite crystal.

The convergence of the operator will be used to draw conclusions about the convergence of eigenvalues similar to that in Holden, Høegh-Krohn and Johannesen [7]. Due to symmetry the formulas will actually be simplified in this case.

First we introduce some notations.

Let Λ be the lattice in $\mathbb{R}^3$, i.e.

$$\Lambda = \{n_1 a_1 + n_2 a_2 + n_3 a_3 | n_i \in \mathbb{Z}\} \tag{3.1}$$

where a_1, a_2, a_3 are three linearly independent vectors in $\mathbb{R}^3$. The orthogonal lattice Γ is

$$\Gamma = \{n_1 b_1 + n_2 b_2 + n_3 b_3 | n_i \in \mathbb{Z}\}$$

where $b_i \in \mathbb{R}^3$ and $a_i \cdot b_j = 2\pi\delta_{ij}$.

We identify the dual group $\hat{\Lambda} = \mathbb{R}^3/\Gamma$ with the Brillouin zone B where

$$B = \{s_1 b_1 + s_2 b_2 + s_3 b_3 | 0 \leq s_i < 1\}. \tag{3.2}$$

Let $\Xi = \{\xi_1, \ldots, \xi_n\}$ be a finite subset of the basic periodic cell Q where

$$Q = \{s_1 a_1 + s_2 a_2 + s_3 a_3 | 0 \leq s_i < 1\} \tag{3.3}$$

Assuming that the potentials V_j, $j = 1,\ldots,n$, are real Rollnik functions with compact support and $\mu_j(\varepsilon)$, $j = 1,\ldots,n$, are real analytic functions around $\varepsilon = 0$ with $\mu_j(0) = 1$, $j = 1,\ldots,n$, we can use lemma 2.1 to define the self-adjoint operator H_ε

$$H_\varepsilon = -\Delta + \sum_{j=1}^{n} \sum_{\lambda\in\Lambda} \varepsilon^{-2}\mu_j(\varepsilon)V_j(\tfrac{1}{\varepsilon}(\cdot-\xi_j-\lambda)). \tag{3.4}$$

From theorem 2.3 we have

$$(H_\varepsilon-E)^{-1} = G_E-\varepsilon C^\varepsilon(1+B^\varepsilon)^{-1}D^\varepsilon \tag{3.5}$$

when $E \notin \sigma(H_\varepsilon)$ and using corollary 2.5 we conclude that

$$(H_\varepsilon-E)^{-1} \overset{n}{\to} (-\Delta^\Lambda_{(\Xi,\alpha)}-E)^{-1} \quad \text{as} \quad \varepsilon \to 0 \tag{3.6}$$

where $-\Delta^\Lambda_{(\Xi,\alpha)}$ is the unique self-adjoint operator on $L^2(\mathbb{R}^3)$ with resolvent

$$(-\Delta^\Lambda_{(\Xi,\alpha)}-E)^{-1} =$$

$$G_E + \sum_{j,\ell=1}^{n} \sum_{\lambda,\lambda'\in\Lambda} |G_E(\cdot-\lambda-\xi_j)\rangle \tag{3.7}$$

$$[(\alpha_j-\frac{i\sqrt{E}}{4\pi})\delta_{j\ell}\delta_{\lambda\lambda'}-\tilde{G}_E(\lambda-\lambda'+\xi_j-\xi_\ell)]^{-1}_{\lambda\lambda' j\ell}\ \langle G_E(\cdot-\lambda'-\xi_\ell)|$$

where $[\ ]^{-1}_{\lambda\lambda' j\ell}$ is the inverse kernel as operator on $\mathbb{C}^n\otimes\ell^2(\Lambda)$ (see Grossmann, Høegh-Krohn and Mebkhout [5] for more details on the limit operator).

Now $\mathcal{H}$ from (2.10) can be identified with

$$\mathcal{H} = L^2(\Lambda,\mathbb{C}^n\otimes L^2(\mathbb{R}^3)). \tag{3.8}$$

The operators B^ε, C^ε and D^ε have kernels

$$D^\varepsilon_{j,\lambda}(x,y) = \mu_j(\varepsilon)u_j(x)G_E(\varepsilon x+\xi_j+\lambda-y) \tag{3.9}$$

$$B^\varepsilon_{j,\ell,\lambda,\lambda'}(x,y) = \varepsilon\mu_j(\varepsilon)u_j(x)G_E(\varepsilon(x-y)+\xi_j-\xi_\ell+\lambda-\lambda')v_\ell(y)$$

$$C^\varepsilon_{j,\lambda}(x,y) = G_E(x-\varepsilon y-\xi_j-\lambda)v_j(y).$$

To simplify (3.5) we use Fourier-analysis on Λ.

We have a natural unitary operator

$$U: L^2(\underline{\underline{R}}^3) \to L^2(\hat{\Lambda}, L^2(Q)) \tag{3.10}$$

where $\hat{\Lambda}$ is to be interpreted as B with its Haar measures, i.e. Lebesque measure divided by $|B|$, the measure of B. U is defined on the Schwartz space S by

$$(Uf)(\theta,\tilde{x}) = \frac{1}{|B|} \sum_{\lambda \in \Lambda} e^{-i\theta\cdot\lambda} f(\tilde{x}+\lambda) \tag{3.11}$$

with $\theta \in B$, $\tilde{x} \in \tilde{Q}$ (see Reed-Simon IV [11]).

Using this operator we have the commutative diagram

$$\begin{array}{ccc} L^2(\underline{\underline{R}}^3) & \xrightarrow{G_E} & L^2(\underline{\underline{R}}^3) \\ U\downarrow & & \downarrow U \\ L^2(\hat{\Lambda}, L^2(Q)) & \xrightarrow{g_E} & L^2(\hat{\Lambda}, L^2(Q)) \end{array} \tag{3.12}$$

where we define the function

$$g_E(x,\theta) = \sum_{\lambda \in \Lambda} G_E(x+\lambda) e^{-i\lambda\cdot\theta} \qquad x \in \underline{\underline{R}}^3,\ \theta \in B \tag{3.13}$$

and the operator g_E by

$$g_E = \int_{\hat{\Lambda}}^{\oplus} g_E(\theta)d\theta \tag{3.14}$$

where $g_E(\theta)$ has integralkernel $g_E(\tilde{x}-\tilde{y},\theta)$, i.e.

$$(g_E(\theta)\psi)(\tilde{x}) = \int_Q g_E(\tilde{x}-\tilde{y},\theta)\psi(\tilde{y})d\tilde{y} \tag{3.15}$$

for $\psi \in L^2(Q)$.

Further we introduce the Fourier transform F with respect to Λ to obtain the following commutative diagrams

$$\begin{array}{ccc} L^2(\underline{\underline{R}}^3) & \xrightarrow{D^\varepsilon} & L^2(\Lambda,\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) \\ U\downarrow & & \downarrow F \\ L^2(\hat{\Lambda},L^2(Q)) & \xrightarrow{\tilde{D}^\varepsilon} & L^2(\hat{\Lambda},\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) \end{array} \tag{3.16}$$

$$\begin{array}{ccc} L^2(\Lambda,\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) & \xrightarrow{B^\varepsilon} & L^2(\Lambda,\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) \\ F\downarrow & & \downarrow F \\ L^2(\hat{\Lambda},\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) & \xrightarrow{\tilde{B}^\varepsilon} & L^2(\hat{\Lambda},\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) \end{array} \tag{3.17}$$

$$\begin{array}{ccc} L^2(\Lambda,\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) & \xrightarrow{C^\varepsilon} & L^2(\underline{\underline{R}}^3) \\ F\downarrow & & \downarrow U \\ L^2(\hat{\Lambda},\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) & \xrightarrow{\tilde{C}^\varepsilon} & L^2(\hat{\Lambda},L^2(Q)) \end{array} \tag{3.18}$$

where

$$\begin{aligned} \tilde{D}^\varepsilon &= \int_{\hat{\Lambda}}^{\oplus} \tilde{D}^\varepsilon(\theta)d\theta \\ \tilde{B}^\varepsilon &= \int_{\hat{\Lambda}}^{\oplus} \tilde{B}^\varepsilon(\theta)d\theta \\ \tilde{C}^\varepsilon &= \int_{\hat{\Lambda}}^{\oplus} \tilde{C}^\varepsilon(\theta)d\theta \end{aligned} \tag{3.19}$$

and

$$(\tilde{D}^{\varepsilon}(\theta)\phi)_j(x) = \mu_j(\varepsilon)u_j(x)\int_Q g_E(\varepsilon x+\xi_j-\tilde{y},\theta)\phi(\tilde{y})d\tilde{y}$$

$$(\tilde{B}^{\varepsilon}(\theta)\psi)_j(x) = \varepsilon\mu_j(\varepsilon)u_j(x)\sum_{\ell=1}^{n}\int_{\underline{\underline{R}}^3} g_E(\varepsilon(x-y)+\xi_j-\xi_\ell,\theta)v_\ell(y)\psi_\ell(y)dy \tag{3.20}$$

$$(\tilde{C}^{\varepsilon}(\theta)\psi)(\tilde{x}) = \sum_{j=1}^{n}\int_{\underline{\underline{R}}^3} g_E(\tilde{x}-\varepsilon y-\xi_j,\theta)v_j(y)\psi_j(y)dy$$

when $\phi \in L^2(Q)$ and $\psi \in \underline{\underline{C}}^n \otimes L^2(\underline{\underline{R}}^3)$.

We want to prove that

$$(1+\tilde{B}^{\varepsilon})^{-1} = \int_{\hat{\Lambda}}^{\oplus}(1+\tilde{B}^{\varepsilon}(\theta))^{-1}d\theta. \tag{3.21}$$

To this end we use the faithful C^*-algebra homomorphism

$$\pi:L^{\infty}(\hat{\Lambda}, (\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3)) \to (L^2(\hat{\Lambda},\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}})) \tag{3.22}$$

(where $\mathcal{B}(\mathcal{H})$ denotes the bounded operators on $\mathcal{H}$) defined by

$$\{A(\theta)\}_{\theta\in\hat{\Lambda}} \overset{\pi}{\mapsto} A = \int_{\hat{\Lambda}}^{\oplus}A(\theta)d\theta. \tag{3.23}$$

From this we have that $1+\tilde{B}^{\varepsilon}$ is invertible in $(L^2(\hat{\Lambda},\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3))$ iff $1+\tilde{B}^{\varepsilon}(\theta)$ is invertible in $(\underline{\underline{C}}^n\otimes L^2(\underline{\underline{R}}^3))$ a.e. and

$$(1+\tilde{B}^{\varepsilon})^{-1} = \int_{\hat{\Lambda}}^{\oplus}(1+\tilde{B}^{\varepsilon}(\theta))^{-1}d\theta. \tag{3.24}$$

Thus we have the following theorem.

<u>Theorem 3.1</u>. We have the integral decomposition

$$UH_{\varepsilon}U^{-1} = \int_{\hat{\Lambda}}^{\oplus}H_{\varepsilon}(\theta)d\theta \tag{3.25}$$

where $H_{\varepsilon}(\theta)$ has resolvent

$$(H_\varepsilon(\theta)-E)^{-1} = g_E(\theta)-\varepsilon\tilde{C}^\varepsilon(\theta)(1+\tilde{B}^\varepsilon(\theta))^{-1}\tilde{D}^\varepsilon(\theta) \tag{3.26}$$

when $E \notin \sigma(H_\varepsilon(\theta))$.

Similar to this decomposition for H_ε we also have one for the operator $-\Delta^\Lambda_{(\Xi,\alpha)}$.

Theorem 3.2. The operator $-\Delta^\Lambda_{(\Xi,\alpha)}$ can be composed in the following way

$$U(-\Delta^\Lambda_{(\Xi,\alpha)})U^{-1} = \int_{\hat{\Lambda}}^{\oplus} -\Delta^\Lambda_{(\Xi,\alpha)}(\theta)d\theta \tag{3.27}$$

where $-\Delta^\Lambda_{(\Xi,\alpha)}(\theta)$ has resolvent

$$(-\Delta^\Lambda_{(\Xi,\alpha)}(\theta)-E)^{-1} = \tag{3.28}$$

$$g_E(\theta)+\sum_{j,\ell=1}^{n}\left[(\alpha_j-\frac{i\sqrt{E}}{4\pi})\delta_{j\ell}-\tilde{g}_E(\xi_j-\xi_\ell,\theta)\right]^{-1}_{j\ell}|g_E(\cdot-\xi_j,\theta)\rangle\langle\overline{g_E(\cdot-\xi_\ell,\theta)}|.$$

Remark. We have defined

$$\tilde{g}_E(x,\theta) = \sum_{\lambda\in\Lambda}\tilde{G}_E(x+\lambda)e^{-i\theta\cdot\lambda} \tag{3.29}$$

where we remember $\tilde{G}_E(x) = G_E(x)$ if $x \neq 0$ and $\tilde{G}_E(0) = 0$. Then we have (see Grossmann, Høegh-Krohn and Mebkhout [5])

$$\tilde{g}_E(x,\theta) = \begin{cases} \dfrac{|B|}{(2\pi)^3}\displaystyle\sum_{\gamma\in\Gamma}\frac{e^{i(\theta+\gamma)\cdot x}}{|\theta+\gamma|^2-E} & \text{if } x\in\Lambda \\ e^{ix\cdot\theta}\left[(2\pi)^{-3}\lim\limits_{\omega\to\infty}(|B|\displaystyle\sum_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\leq\omega}}\frac{1}{|\theta+\gamma|^2-E}-4\pi\omega)-\frac{i\sqrt{E}}{4\pi}\right] & \text{if } x\in\Lambda \end{cases} \tag{3.30}$$

Proof: In Grossmann, Høegh-Krohn and Mebkhout [5] the operator $-\Delta^\Lambda_{(\Xi,\alpha)}$ is decomposed in p-space. We denote the p-space version of $-\Delta^\Lambda_{(\Xi,\alpha)}$ considered on $L^2(\hat{\Lambda},l^2(\Gamma))$ by $-\Delta_\alpha$. Then we have

$$-\Delta_\alpha = \int_{\hat{\Lambda}}^{\oplus} -\Delta_\alpha(\theta)d\theta \tag{3.31}$$

where $-\Delta_\alpha(\theta)$ is an operator on $l^2(\Gamma)$ whose resolvent has integral kernel given by

$$(-\Delta_\alpha(\theta)-E)^{-1}_{\gamma\gamma'} = \tag{3.32}$$

$$(|\gamma+\theta|^2-E)^{-1}\delta_{\gamma\gamma'}+(2\pi)^{-3}\sum_{j,\ell=1}^{n}[(\alpha_j-\frac{i\sqrt{E}}{4\pi})\delta_{j\ell}-\tilde{g}_E(\xi_j-\xi_\ell,\theta)]^{-1}_{j\ell}$$

$$\frac{e^{-i(\gamma+\theta)\cdot\xi_j}}{|\gamma+\theta|^2-E}\cdot\frac{e^{i(\gamma'+\theta)\cdot\xi_\ell}}{|\gamma'+\theta|^2-E}.$$

Defining the operator S by

$$S: L^2(\hat{\Lambda}, l^2(\Gamma)) \to L^2(\hat{\Lambda}, L^2(Q)) \tag{3.33}$$

and

$$(S\psi)(\theta,\tilde{x}) = (2\pi)^{-3/2}\sum_{\gamma\in\Gamma}\psi(\theta,\gamma)e^{i(\theta+\gamma)\cdot\tilde{x}} \tag{3.34}$$

when $\psi \in L^2(\hat{\Lambda}, l^2(\Gamma))$ we can show that the following diagram commutes:

$$\begin{array}{ccc} L^2(\hat{\Lambda},l^2(\Gamma)) & \xrightarrow{\tilde{g}_E} & L^2(\hat{\Lambda},l^2(\Gamma)) \\ S\downarrow & & \downarrow S \\ L^2(\hat{\Lambda},L^2(Q)) & \xrightarrow{g_E} & L^2(\hat{\Lambda},L^2(Q)) \end{array} \tag{3.35}$$

where

$$\tilde{g}_E = \int_{\hat{\Lambda}}^{\oplus}\tilde{g}_E(\theta)d\theta \tag{3.36}$$

(this $\tilde{g}_E$ is not to be confused with the $\tilde{g}_E(x,\theta)$ defined by (3.29)) and

$$\tilde{g}_E(\theta)_{\gamma\gamma'} = (|\gamma+\theta|^2-E)^{-1}\delta_{\gamma\gamma'}. \tag{3.37}$$

Using this operator we obtain the stated decomposition.

Theorem 3.3. The decomposed operator $H_\varepsilon(\theta)$ converges in norm resolvent sense to $-\Delta^{\Lambda}_{(\Xi,\alpha)}(\theta)$ as $\varepsilon \to 0$ when $\alpha = (\alpha_1,\ldots,\alpha_n)$ is given according to

$$\alpha_j = \mu_j'(0)(\tilde{\phi}_j,\phi_j)|(v_j,\phi_j)|^{-2}. \tag{3.38}$$

Proof: The proof is identical to that of theorem 2.5 in Holden, Høegh-Krohn and Johannesen [7] except that one has to replace G_E by g_E.

By this decomposition we have in the standard way reduced the band spectrum of H_ε and $-\Delta^{\Lambda}_{(\Xi,\alpha)}$ to isolated eigenvalues for each operator $H_\varepsilon(\theta)$ and $-\Delta^{\Lambda}_{(\Xi,\alpha)}(\theta)$ when $\theta \in \hat{\Lambda}$. The union over all eigenvalues for all $\theta \in \hat{\Lambda}$ gives the spectrum of H_ε and $-\Delta^{\Lambda}_{(\Xi,\alpha)}$.

We now want to use the norm resolvent convergence to expand in ε the eigenvalues of $-H_\varepsilon(\theta)$.

To simplify matters we first study the one center case, i.e. $|\Xi| = 1$, and we can assume $\Xi = \{0\}$ without loss of generality. In this case the spectrum is completely described by the following theorem. We put $-\Delta^{\Lambda}_{\alpha} \equiv -\Delta^{\Lambda}_{\{0\},\alpha}$ and similarly $-\Delta^{\Lambda}_{\alpha}(\theta) = -\Delta^{\Lambda}_{\{0\},\alpha}(\theta)$.

Theorem 3.4.

(a) $-\Delta^{\Lambda}_{\alpha}(\theta)$ has pure point spectrum and E^θ is an eigenvalue for $-\Delta^{\Lambda}_{\alpha}(\theta)$ with multiplicity m iff

$$\text{(I)} \quad \alpha = g_E\theta(0,\theta) \quad \text{and} \quad m = 1 \tag{3.39}$$

or

(II) There exist m+1 points $\gamma_0,\ldots,\gamma_m \in \Gamma$ such that

$$E^{\theta} = |\gamma_0+\theta|^2 = \ldots = |\gamma_m+\theta|^2 \qquad (3.40)$$

(b) The spectrum of $-\Delta_{\alpha}^{\Lambda}$ is absolutely continuous and there exist numbers $E_0(\alpha)$, $E_1(\alpha)$ such that

$$\sigma(-\Delta_{\alpha}^{\Lambda}) = [E_0(\alpha),E_1(\alpha)] \cup [0,\infty) \qquad (3.41)$$

$E_1(\alpha) < 0$ iff $\alpha < \alpha_0 < 0$ where α_0 is given in [5].

<u>Proof</u>: See Grossmann, Høegh-Krohn and Mebkhout [5].

<u>Remark</u>. We observe that the negative eigenvalues are all in case (I).

We can now prove the following theorem.

<u>Theorem 3.5</u>. Assume that $z^{\theta}(\varepsilon)$ is an eigenvalue for $H_{\varepsilon}(\theta)$ for $\varepsilon > 0$ which remains bounded for small positive ε.

Let $\{\varepsilon_n\}$ be a positive sequence decreasing to zero and let E_0^{θ} be an accumulation point for $\{z^{\theta}(\varepsilon_n)\}$.

Then E_0^{θ} is an eigenvalue for $-\Delta_{\alpha}^{\Lambda}(\theta)$. Assume that this eigenvalue is in case (I). Then we have that if $E_0^{\theta} < 0$ $(E_0^{\theta} \geq 0)$ there exists an analytic (differentiable) function $E^{\theta}(\varepsilon)$ in ε such that $E^{\theta}(\varepsilon)$ is an eigenvalue for $H_{\varepsilon}(\theta)$ and we have

$$E^{\theta}(\varepsilon) = E_0^{\theta}+\varepsilon E_1^{\theta}+o(\varepsilon) \qquad (3.42)$$

where

$$E_1^{\theta} = h_{\Lambda}^{\theta}(A+E_0^{\theta}B) \qquad (3.43)$$

where A, B and h_{Λ}^{θ} are given by

$$A = \mu'(0)(\tilde{\phi},\phi')-\alpha(v,\phi)+\tfrac{1}{2}\mu''(0)\alpha-\mu'(0)\alpha \qquad (3.44)$$

$$B = \frac{1}{8\pi} \iint \phi(x)v(x)|x-y|v(y)\phi(y)dxdy \qquad (3.45)$$

and

$$h_\Lambda^\theta = (2\pi)^3 [|B| \sum_{\gamma\in\Gamma} \frac{1}{(|\gamma+\theta|^2 - E_0^\theta)^2}]^{-1} \tag{3.46}$$

Remarks. 1. The formula for E_1^θ has a surprising simplicity. The terms A and B are independent of the lattice and depends only on the properties of one point without any lattice. The lattice dependence is only the term h_Λ^θ.

From the analysis in Grossmann, Høegh-Krohn and Mebkhout [5] we know that each eigenvalue E^θ in case (I) for $-\Delta_\alpha^\Lambda(\theta)$ gives rise to a band when θ varies. The bands are connected at points E^θ where there are at least three points $\gamma_1, \gamma_2, \gamma_3 \in \Gamma$ with $E^\theta |= \gamma_1+\theta|^2 = |\gamma_2+\theta|^2 = |\gamma_3+\theta|^2$.

If we now let E^{θ_0} be such a point of connection and let $\theta \to \theta_0$ with E^θ in case (I) we see from (3.43) that $E_1^\theta \to 0$. Thus in this sense we have that the bands do not dissolve to first order.

2. Expanding B to higher order makes it possible to obtain formulas to the next order of $E^\theta(\varepsilon)$. However the formulas do not have the same simplicity as the first one.

Proof: From the norm resolvent convergence we conclude that E_0^θ is an eigenvalue for $-\Delta_\alpha^\Lambda(\theta)$.

Case (i). $E_0^\theta < 0$.

Then $z^\theta(\varepsilon_n) < 0$ which implies that the pole of the resolvent of $H_\varepsilon(\theta)$ has to come from $(1+\tilde{B}^\varepsilon(\theta))^{-1}$, i.e. -1 is an eigenvalue for $\tilde{B}^\varepsilon(\theta)$.

The proof now closely follows the proof of theorem 3.1 in Holden, Høegh-Krohn and Johannesen [7], so we will sketch this part.

We expand the operator $1+\tilde{B}_E^\varepsilon(\theta)$ in ε where we have introduced the E dependence in the operator defined by (3.20), i.e.

$$1+\tilde{B}_E^\varepsilon(\theta) = 1+S+\varepsilon T+O(\varepsilon) \tag{3.47}$$

where

$$S = uG_0 v \tag{3.48}$$

and

$$T = \mu'(0)uG_0 v+(\frac{i\sqrt{E}}{4\pi} +\tilde{g}_E(0,\theta)\,|u\rangle\langle v|\,. \tag{3.49}$$

We split the space $L^2(\underline{\underline{R}}^3)$ into H_0 and H_1, i.e.

$$L^2(\underline{\underline{R}}^3) = H_0 \dot{+} H_1 \tag{3.50}$$

where

$$H_0 = \mathrm{Ker}(1+S), \quad H_1 = \mathrm{Ran}(1+S). \tag{3.51}$$

Then

$$P = \frac{|\phi\rangle\langle\tilde{\phi}|}{(\tilde{\phi},\phi)} \tag{3.52}$$

is a projection onto H_0.

This enables us to write $\tilde{B}_E^\varepsilon(\theta)$ in the following way

$$\tilde{B}_E^\varepsilon(\theta) = \begin{bmatrix} -1+\varepsilon T_{00}+o_{00}(\varepsilon) & \varepsilon T_{01}+o_{01}(\varepsilon) \\ \varepsilon T_{10}+o_{10}(\varepsilon) & S_{11}+\varepsilon T_{11}+o_{11}(\varepsilon) \end{bmatrix} \tag{3.53}$$

where we have

$$T_{00}= PTP,\ T_{10}= (1-P)TP,\ T_{01}= PT(1-P) \text{ and } T_{11}= (1-P)T(1-P) \tag{3.54}$$

and similarly for $S(\varepsilon)$ and $o(\varepsilon)$.

We now introduce the operator $\mathcal{B}_E^\varepsilon(\theta)$ defined by

$$\mathcal{B}_E^\varepsilon(\theta) = \begin{bmatrix} -1+T_{00}+\frac{1}{\varepsilon}o_{00}(\varepsilon) & \varepsilon T_{01}+o_{01}(\varepsilon) \\ T_{10}+\frac{1}{\varepsilon}o_{10}(\varepsilon) & S_{11}+\varepsilon T_{11}+o_{11}(\varepsilon) \end{bmatrix} \tag{3.55}$$

Then one can deduce that when $\varepsilon > 0$

$$-1 \in \sigma(\mathcal{B}_E^{\varepsilon}(\theta)) \iff -1 \in \sigma(\tilde{B}_E^{\varepsilon}(\theta)) \tag{3.56}$$

and the operator $\mathcal{B}_E^{\varepsilon}(\theta)$ has the advantage that when $\varepsilon = 0$, $\mathcal{B}_E^{0}(\theta)$ depends on E and θ while $\tilde{B}_E^{0}(\theta) = S$ is independent of both E and θ.

This fact together with (3.56) makes it possible to use implicit function theory on the function

$$d(\theta,\varepsilon,E) = \det_2(1+\mathcal{B}_E^{\varepsilon}(\theta)) \tag{3.57}$$

where $\det_2$ denotes the modified Fredholm-determinant (see e.g. Simon [12]).

Putting $\varepsilon = 0$ in (3.57) we obtain

$$\begin{aligned} d(\theta,0,E) &= \det_2 \begin{bmatrix} 1+(T_{00}-1) & 0 \\ T_{10} & 1+S_{11} \end{bmatrix} \\ &= \det_2 \begin{bmatrix} 1+(T_{00}-1) & 0 \\ T_{10} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1+S_{11} \end{bmatrix} \\ &= \det_2 \begin{bmatrix} 1+(T_{00}-1) & 0 \\ T_{10} & 1 \end{bmatrix} \det_2 \begin{bmatrix} 1 & 0 \\ 0 & 1+S_{11} \end{bmatrix} \\ &= \det_2 (T_{00}) \det_2 (1+S_{11}) \\ &= \det (T_{00}) e^{-\mathrm{Tr}(T_{00}-1)} \det_2(1+S_{11}) \end{aligned} \tag{3.58}$$

Now $\det_2(1+S_{11})$ is independent of θ, E and the other terms except the first are never zero.

We have:

$$\det T_{00} = -\frac{1}{(\tilde{\phi},\phi)} \left[\alpha - \frac{i\sqrt{E}}{4\pi} - \tilde{g}_E(0,\theta)\right] \tag{3.59}$$

when we have normalized ϕ such that $(v,\phi) = 1$.

This implies that

$$\frac{\partial}{\partial E} d(\theta, 0, E_0^\theta) \neq 0 \tag{3.60}$$

Thus by the implicit function theorem we obtain an analytic function $E^\theta(\varepsilon)$ with $E^\theta(0) = E_0^\theta$ and

$$d(\theta, \varepsilon, E^\theta(\varepsilon)) = 0 \tag{3.61}$$

i.e. $E^\theta(\varepsilon)$ is an eigenvalue for $H_\varepsilon(\theta)$.

Returning to $\tilde{B}^\varepsilon_{E^\theta(\varepsilon)}(\theta)$ we have an analytic operator with -1 as a simple eigenvalue when ε is small.

Then there exists an eigenvector ϕ_θ^ε such that $\varepsilon \mapsto \phi_\theta^\varepsilon$ is analytic and

$$(1+\tilde{B}^\varepsilon_{E^\theta(\varepsilon)}(\theta))\phi_\theta^\varepsilon = 0. \tag{3.62}$$

Expanding $\tilde{B}^\varepsilon_{E^\theta(\varepsilon)}(\theta)$ and ϕ^ε in powers of ε we obtain

$$(1+uG_0v)\phi = 0 \tag{3.63}$$

to zeroth order where $\phi = \phi_\theta^0$ is independent of θ. We normalize ϕ such that $(\phi, v) = 1$. To first order we have

$$(1+uG_0v)\phi_\theta' = \mu'(0)\phi - \alpha u \tag{3.64}$$

which implies that

$$\phi_\theta' = c_\theta\phi + (1+uG_0v)\big|^{-1}_{\mathrm{Ran}(1+uG_0v)}(\mu'(0)\phi - \alpha u) \tag{3.65}$$

where c_θ is a constant. To second order we have when we take inner-product with $\tilde{\phi} = \phi \operatorname{sgn} V$ that

$$2\alpha(v,\phi') - 2\mu'(0)(\tilde{\phi},\phi') + 2\mu'(0)\alpha - \mu''(0)\alpha \tag{3.66}$$

$$- \frac{E_0^\theta}{4\pi}\int\int \phi(x)v(x)|x-y|v(y)\phi(y)\,dx\,dy + 2E_1^\theta \frac{|B|}{(2\pi)^3}\sum_{\gamma\in\Gamma}\frac{1}{(|\gamma+\theta|^2 - E_0^\theta)^2} = 0$$

where

$$\phi' = (1+uG_0v)|^{-1}_{\mathrm{Ran}(1+uG_0v)}(\mu'(0)\phi-\alpha u). \tag{3.67}$$

Defining

$$A = \mu'(0)(\tilde{\phi},\phi')-\alpha(v,\phi')+\tfrac{1}{2}\mu''(0)\alpha-\mu'(0)\alpha \tag{3.68}$$

$$B = \frac{1}{8\pi}\iint\phi(x)v(x)|x-y|v(y)\phi(y)dxdy \tag{3.69}$$

and

$$h^{\theta}_{\Lambda} = (2\pi)^3[|B|\sum_{\gamma\in\Gamma}\frac{1}{(|\gamma+\theta|^2-E^{\theta}_0)^2}]^{-1} \tag{3.70}$$

we obtain the stated expansion (3.42).

<u>Case (ii)</u>. $E^{\theta}_0 \geqslant 0$ and E^{θ}_0 is in case (I).

Then $E^{\theta}_0 \neq |\gamma+\theta|^2$ for all $\gamma \in \Gamma$ which implies that $z^0_{\varepsilon} \neq |\gamma+\theta|^2$ for all $\gamma \in \Gamma$ thus making a pole of $(1+\tilde{B}^{\varepsilon}_E(\theta))^{-1}$.

We now follow the same argument as in case (i) except now we cannot say that $\tilde{B}^{\varepsilon}_E(\theta)$ and thus $B^{\varepsilon}_E(\theta)$ is analytic.

We have that $\tilde{B}^{\varepsilon}_E(\theta)$ is a C^2 operator-valued function in ε when $E \geqslant 0$.

Following Kato [8] the projection $P(\varepsilon)$ onto the eigenspace corresponding to the eigenvalue -1 of $\tilde{B}^{\varepsilon}_E(\theta)$ is a C^2 function in ε.

Defining $\phi^{\varepsilon}_{\theta} = P^{\theta}(\varepsilon)\phi$ where ϕ is an eigenfunction for $\tilde{B}^0_E(\theta)$ we obtain (3.62) which can be expanded sufficiently to give the equation (3.66) for E^{θ}_1.

Also in the general case with n centers par lattice site one is able to give some properties of the spectrum in the limit when $\varepsilon = 0$.

We recall the following theorem ($|\Xi|$ is the number of points in the set Ξ).

Theorem 3.6. Let $n = |\Xi|$. Then $\sigma(\Delta^{\wedge}_{(\Xi,\alpha)}) \cap (-\infty,0)$ consists of at most n disjoint intervals.

Proof: See Høegh-Krohn, Holden and Martinelli [6].

Again we can state a theorem concerning the convergence of the negative eigenvalues of the decomposed operators.

Theorem 3.7. Assume that $z^{\theta}(\varepsilon)$ is an eigenvalue for $H_{\varepsilon}(\theta)$ such that $-\infty < M_1 \leq z^{\theta}(\varepsilon) \leq M_2 < 0$ when $\varepsilon > 0$ is small.

Let $\{\varepsilon_n\}$ be a positive sequenze decreasing to zero and let E_0^{θ} be an accumulation point for $\{z^{\theta}(\varepsilon_n)\}_n$.

Then E_0^{θ} is an eigenvalue for $-\Delta^{\wedge}_{(\Xi,\alpha)}(\theta)$. Let m be its multiplicity.

Then we have:

There exist m multivalued analytic functions $E_1^{\theta}(\varepsilon),\ldots,E_m^{\theta}(\varepsilon)$ with $E_j^{\theta}(0) = E_0^{\theta}$ such that $E_j^{\theta}(\varepsilon)$ is an eigenvalue for $H_{\varepsilon}(\theta)$ and we have

$$E_j^{\theta}(\varepsilon) = E_0^{\theta}+\varepsilon^{1/m}E_{j,1}^{\theta}+o(\varepsilon^{1/m}) \tag{3.71}$$

where $E_{j,1}^{\theta}$ is given by (3.43) when $m = 1$ and is a solution of (3.82) when $m > 1$.

Proof: We closely follow the strategy of the proof of theorem 3.5. Expanding $1+\tilde{B}_E^{\varepsilon}(\theta)$ in ε we obtain:

$$1+\tilde{B}_E^{\varepsilon}(\theta) = 1+S+\varepsilon T+o(\varepsilon) \tag{3.72}$$

where now

$$S = [\delta_{j\ell}u_j G_0 v_j] \tag{3.73}$$

$$T = [(\mu_j'(0)u_j G_0 v_j + \frac{i\sqrt{E}}{4\pi}|u_j\rangle\langle v_j|)\delta_{j\ell}+\tilde{g}_E(\xi_j-\xi_\ell,\theta)|u_j\rangle\langle v_\ell|]$$

We split $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\underline{\underline{R}}^3)$ into $\mathcal{H}_0 = \mathrm{Ker}(1+S)$ and $\mathcal{H}_1 = \mathrm{Ran}(1+S)$, i.e.

$$\mathcal{H} = \mathcal{H}_0 \dot{+} \mathcal{H}_1 . \tag{3.74}$$

Now

$$P = [\delta_{j\ell} \frac{|\phi_j><\tilde{\phi}_j|}{(\tilde{\phi}_j,\phi_j)}] \tag{3.75}$$

is a projection onto $\mathcal{H}_0$.

Using this decomposition to define the operator $\mathcal{B}_E^{\varepsilon}(\theta)$ as in (3.55) we have with

$$d(\theta,\varepsilon,E) = \det{}_2(1+\mathcal{B}_E^{\varepsilon}(\theta)) \tag{3.76}$$

that

$$d(\theta,o,E) = \det T_{00} \det{}_2(1+S_{11}) e^{-\mathrm{Tr}(T_{00}-1)} \tag{3.77}$$

and in this case

$$\det T_{00} = (-1)^n \frac{1}{(\tilde{\phi}_1,\phi_1)\ldots(\tilde{\phi}_n,\phi_n)} \det[(\alpha_j - \frac{i\sqrt{E}}{4\pi})\delta_{jl} - \tilde{g}_E(\xi_j-\xi_l,\theta)]. \tag{3.78}$$

The explicit expression (3.78) implies the existence of m (where m is the multiplicity of the eigenvalue E_0^{θ} of $-\Delta_{(\Xi,\alpha)}(\theta)$) not necessarily different multivalued analytic functions $E_1^{\theta}(\varepsilon),\ldots,E_m^{\theta}(\varepsilon)$ with $E_j^{\theta}(0) = E_0^{\theta}$, i.e.

$$E_j^{\theta}(\varepsilon) = E_0^{\theta} + g_j^{\theta}(\varepsilon^{1/m}) \tag{3.79}$$

where g_j^{θ} is analytic, $g_j^{\theta}(0) = 0$.

Considering the operator $\tilde{\mathcal{B}}^{\varepsilon^m}_{E_j^{\theta}(\varepsilon^m)}(\theta)$ we have an analytic operator with constant eigenvalue -1.

Then there exists (see the proof of theorem 3.1 in Holden, Høegh-Krohn and Johannesen [7]) an analytic eigenvector such that

$$(1+\tilde{B}^{\varepsilon^m}_{E^\theta_j(\varepsilon^m)}(\theta))\phi^\varepsilon_\theta = 0. \tag{3.80}$$

When $m = 1$ we get the same formula for $E^\theta_1 = \frac{dE^\theta(\varepsilon)}{d\varepsilon}\Big|_{\varepsilon=0}$ as before, i.e.

$$E^\theta_1 = h^\theta_\Lambda(A+E^\theta_0 B). \tag{3.81}$$

When $m > 1$ we obtain by taking the derivative in (3.80) m+1 times that $\dot{E}^\theta_1$, the derivative of the function $E^\theta_j(\varepsilon^n)$, is a solution of the system of equations:

$$\begin{aligned} & E^\theta_1(\phi^0_j,v_j)\sum_{\ell=1}^n \frac{|B|}{(2\pi)^3}\Big(\sum_{\gamma\in\Gamma}\frac{e^{i(\theta+\gamma)\cdot(\xi_j-\xi_\ell)}}{(|\theta+\gamma|^2-E^\theta_0)^2}\Big)(v_\ell,\phi^0_\ell) \\ & - \mu'_j(0)(\tilde{\phi}^0_j,\phi'_j) + \frac{i\sqrt{E^\theta_0}}{4\pi}(\phi^0_j,v_j)(v_j,\phi'_j) \\ & + (\phi^0_j,v_j)\sum_{\ell=1}^n \tilde{g}_{E^\theta_0}(\xi_j-\xi_\ell,\theta)(v_\ell,\phi'_\ell) = 0 \end{aligned} \tag{3.82}$$

for $j = 1,\ldots,n$ where $((v_1,\phi^0_1),\ldots,(v_n,\phi^0_n))$ fullfills

$$\sum_{\ell=1}^n \Big[\Big(\alpha_j - \frac{i\sqrt{E^\theta_0}}{4\pi}\Big)\delta_{j\ell} - \tilde{g}_{E^\theta_0}(\xi_j-\xi_\ell,\theta)\Big](v_\ell,\phi^0_\ell) = 0$$

and

$$(1+u_j G_0 V_j)\phi'_j = 0$$

for $j = 1,\ldots,n$.

4. Infinite straight polymers.

In this section we replace the lattice $\Lambda = \{n_1 a_1 + n_2 a_2 + n_3 a_3 | a_i \in \mathbb{Z}\}$ from section 3 with the discrete abelian subgroup $\Lambda = \{(0,0,na) \in \mathbb{R}^3 | n \in \mathbb{Z}\}$ where $a > 0$. This then, is a model of an infinite straight polymer.

Let furthermore $\Xi = \{\xi_1, \dots, \xi_n\}$ be a finite subset of $\mathbb{R}^3$ with $0 \leq \xi_i^3 < a$ where $\xi_i = (\xi_i^1, \xi_i^2, \xi_i^3)$. Then we can define the self-adjoint operator

$$H_\varepsilon = -\Delta + \sum_{j=1}^{n} \sum_{\lambda \in \Lambda} \varepsilon^{-2} \mu_j(\varepsilon) V_j(\tfrac{1}{\varepsilon}(\cdot - \xi_j - \lambda)) \tag{4.1}$$

where V_j are Rollnik functions with compact support and μ_j are analytic function with $\mu_j(0) = 1$, and we know from corollary 2.5 that this operator converges in norm resolvent sense to the operator $-\Delta_{(\Xi,\alpha)}$ with resolvent

$$(-\Delta_{(\Xi,\alpha)} - E)^{-1} = G_E + \sum_{j,\ell=1}^{n} \sum_{\lambda,\lambda' \in \Lambda} [(\alpha_j - \frac{i\sqrt{E}}{4\pi})\delta_{j\ell}\delta_{\lambda\lambda'} - \tilde{G}_E(\lambda - \lambda' + \xi_j - \xi_\ell)]^{-1}_{j\ell\lambda\lambda'}$$

$$|G_E(\cdot - \lambda - \xi_j)\rangle\langle G_E(\cdot - \lambda' - \xi_\ell)| \tag{4.2}$$

when

$$\alpha_j = \mu_j'(0)(\tilde{\phi}_j, \phi_j)|(v_j, \phi_j)|^{-2}. \tag{4.3}$$

To study the spectral properties with this approximation we simplify to the case when $|\Xi| = 1$ and again we can assume that $\Xi = \{0\}$. We denote $-\Delta_{(\{0\},\alpha)}$ by $-\Delta_\alpha^\Lambda$ and similarly for the decomposed operator. From theorem 2.3 we have that

$$(H_\varepsilon - E)^{-1} = G_E - \varepsilon C^E (1 + B^\varepsilon)^{-1} D^\varepsilon \tag{4.4}$$

and again we use Fourier-analysis to analyse the spectrum.

The analysis is quite similar to that of the model of the crystal so we will sketch this part.

Considering H_ε as an operator on $L^2(\hat{\Lambda}, L^2(\underline{\underline{R}}^2) \otimes L^2(Q))$ where $Q = [0,a)$ and $\hat{\Lambda}$ is identified with $[-\frac{\pi}{a}, \frac{\pi}{a})$ with Haar-measure we can decompose H_ε

$$H_\varepsilon = \int_{\hat{\Lambda}}^{\oplus} H_\varepsilon(\theta) d\theta \tag{4.5}$$

where $H_\varepsilon(\theta)$ has resolvent

$$(H_\varepsilon(\theta) - E)^{-1} = g_E(\theta) - \varepsilon \tilde{C}^\varepsilon(\theta)(1 + \tilde{B}^\varepsilon(\theta))^{-1} \tilde{D}^\varepsilon(\theta). \tag{4.6}$$

The operators $g_E(\theta)$, $\tilde{C}^\varepsilon(\theta)$, $\tilde{B}^\varepsilon(\theta)$ and $\tilde{D}^\varepsilon(\theta)$ have integral kernels given by

$$\begin{aligned}
g_E(\theta)((x_1,x_2,\tilde{x}),(y_1,y_2,\tilde{y})) &= g_\varepsilon((x_1,x_2\tilde{x})-(y_1,y_2,\tilde{y}),\theta) \\
\tilde{C}^\varepsilon(\theta)((x_1,x_2,\tilde{x}),y) &= g_\varepsilon((x_1,x_2,\tilde{x})-\varepsilon y,\theta)v(y) \\
\tilde{B}^\varepsilon(\theta)(x,y) &= \varepsilon\mu(\varepsilon)u(x)g_E(\varepsilon(x-y),\theta)v(y) \\
\tilde{D}^\varepsilon(\theta)(x,(y_1,y_2,\tilde{y})) &= \mu(\varepsilon)u(x)g_\varepsilon(\varepsilon x-(y_1,y_2,\tilde{y}),\theta)
\end{aligned} \tag{4.7}$$

where $x_1,x_2,y_1,y_2 \in \underline{\underline{R}}$, $\tilde{x},\tilde{y} \in Q$ and

$$g_E(x,\theta) = \sum_{\lambda \in \Lambda} G_E(x+\lambda)e^{-i\theta \cdot \lambda}. \tag{4.8}$$

In Grossmann, Høegh-Krohn and Mebkhout [5] the operator $-\Delta_\alpha^\Lambda$ is decomposed in p-space.

By making essentially a Fourier-transform we obtain a decomposition of $-\Delta_\alpha^\Lambda$ considered on $L^2(\hat{\Lambda}, L^2(\underline{\underline{R}}^2) \otimes L^2(Q))$

$$-\Delta_\alpha^\Lambda = \int_{\hat{\Lambda}}^{\oplus} -\Delta_\alpha^\Lambda(\theta) d\theta \tag{4.9}$$

where

$$(-\Delta_\alpha^\Lambda(\theta)-E)^{-1} = g_E(\theta)+[\alpha-\frac{i\sqrt{E}}{4\pi}-\tilde{g}_E(0,\theta)]^{-1}|g_E(\cdot,\theta)\rangle\langle\overline{g_E(\cdot,\theta)}| \quad (4.10)$$

and

$$\begin{aligned}\tilde{g}_E(0,\theta) &= \sum_{\substack{\lambda\in\Lambda\\ \lambda\neq 0}} G_E(\lambda)e^{-i\theta\cdot\lambda}\\ &= -\frac{1}{4\pi a}\ln 2\ (\cos\sqrt{E}a-\cos\theta a) - \frac{i\sqrt{E}}{4\pi}.\end{aligned} \quad (4.11)$$

Again we have

<u>Theorem 4.1</u>. The operator $H_\varepsilon(\theta)$ converges in norm resolvent sense to $-\Delta_\alpha(\theta)$ when $\varepsilon \to 0$ and α is given according to (4.3).

<u>Proof</u>: Similar to that of theorem 2.5 in Holden, Høegh-Krohn and Johannesen [7].

Using this theorem we could procede as in section 3 to expand the eigenvalues in ε. However this model of an infinite straight polymer has one property which is not shared by the model for the crystal, namely real resonances on which we will concentrate here. Concerning the real resonances of $-\Delta_\alpha$ we have

<u>Theorem 4.2</u>. If $\alpha > -\frac{\ln 2}{2\pi a}$ there exists at least one $\theta \in \hat{\Lambda}$ such that $-\Delta_\alpha(\theta)$ has an infinite number of simple real resonances

$$E_n^\theta = \frac{1}{a^2}(\arccos(\cos\theta+\tfrac{1}{2}e^{-4\pi a\alpha})+2\pi n)^2 \quad (4.12)$$

when $n \in \underline{\underline{N}}$.

<u>Proof</u>: From (4.10) we see that resonances and eigenvalues are solutions of

$$\cos\sqrt{E}a = \cos\theta a+\tfrac{1}{2}e^{-4\pi a\alpha}. \quad (4.13)$$

From the assumption $\alpha > -\frac{\ln 2}{2\pi a}$ we can infer the existence of at least one θ such that

$$\cos\ \theta+\tfrac{1}{2}e^{-4\pi a\alpha} < 1$$

which implies that

$$E = \frac{1}{a^2}(\arccos(\cos\theta+\tfrac{1}{2}e^{-4\pi a\alpha})+2\pi n)^2, \quad n \in N.$$

In Grossmann, Høegh-Krohn and Mebkhout [5] it is argued why these are resonances and not eigenvalues.

<u>Theorem 4.3</u>. Let $\alpha \geqslant -\frac{\ln 2}{2\pi a}$ and let θ be according to theorem 4.2 and $E_n(\theta)$ be defined by (4.12). Then for $\varepsilon > 0$ small $H_\varepsilon(\theta)$ has a simple resonance $E_n^\theta(\varepsilon)$ such that

$$E_n^\theta(\varepsilon) = E_n^\theta+\varepsilon E_{n,1}^\theta+o(\varepsilon)$$

where

$$E_{n,1}^\theta = \frac{4\pi\sqrt{E_n^\theta}(\cos\sqrt{E_n^\theta}a-\cos\theta a)}{\sin\sqrt{E_n^\theta}a}(A+E_n^\theta B)$$

and A,B are given by (3.44), (3.45) respectively.

<u>Proof</u>: The proof follows that of theorem 3.5, except for the fact that we have to argue that the resonance for $-\Delta_\alpha(\theta)$ has not turned into an eigenvalue. But from the norm resolvent convergence this is impossible.

<u>Remark</u>. By observing that the formula for $E_{n,1}^\theta$ gives a real number we have that the resonance is real also to first order in ε.

5. Mono-molecular layer.

We can of course also use the methods utilized in section 3 and 4 to study a model of a mono-molecular layer, i.e. to define Λ as

$$\Lambda = \{n_1 a_1 + n_2 a_2 \,|\, n_i \in \mathbb{Z}\} \tag{5.1}$$

where $a_i = (a_i^1, a_i^2, 0) \in \mathbb{R}^3$ $i = 1,2$ and a_1 and a_2 are linearly independent.

Again we get the same structure of the eigenvalues to first order, i.e.

$$E_1^\theta = h_\Lambda^\theta (A + E_0^\theta B) \tag{5.2}$$

where A, B are as usual given by (3.44) and (3.45) and h_Λ^θ is a term depending on the Λ considered. In the case of a mono-molecular layer, i.e. when Λ is given by (5.1) we have that

$$h_\Lambda^\theta = (2\pi)^3 \Big[\frac{1}{4}|B| \sum_{\gamma \in \Gamma} ((\gamma^1+\theta^1)^2 + (\gamma^2+\theta^2)^2 - E)^{-3/2}\Big]^{-1} \tag{5.3}$$

where $\Gamma = \{n_1 b_1 + n_2 b_2 \,|\, n_i \in \mathbb{Z}\}$ is the orthogonal lattice, i.e. $a_i \cdot b_j = 2\pi\delta_{ij}$ and $\gamma = (\gamma^1, \gamma^2, 0) \in \Gamma$.

The dual group $\hat{\Lambda}$ is identified with the Brillouin zone B where

$$B = \{s_1 b_1 + s_2 b_2 \,|\, 0 \leqslant s_i < 1\} \tag{5.4}$$

and $\theta = (\theta^1, \theta^2, \theta^3) \in B$.

We omit the details.

Appendix.

In this appendix we will define the so-called Holmgren-norm.

Let $\{H_n\}$ be a sequenze of Hilbert-spaces and define

$$H = \bigoplus_{n=1}^{\infty} H_n .$$

Let further $A = [A_{ij}]$ be an operator on H with $D(A) = H$. If $\phi = (\phi_n) \in H$ we have

$$\|A\phi\|^2 = \sum_i \|\sum_j A_{ij}\phi_j\|^2 \leqslant \sum_i (\sum_j \|A_{ij}\| \sum_j \|A_{ij}\|\|\phi_j\|^2)$$

$$\leqslant \sup_i \sum_j \|A_{ij}\| \sum_j (\sum_i \|A_{ij}\|\|\phi_j\|^2)$$

$$\leqslant \sup_i \sum_j \|A_{ij}\| \sup_j \sum \|A_{ij}\| \sum_j \|\phi_j\|^2$$

$$\leqslant \|A\|_H^2 \|\phi\|^2$$

where

$$\|A\|_H \equiv (\sup_i \sum_j \|A_{ij}\| \sup_j \sum_i \|A_{ij}\|)^{\frac{1}{2}}$$

is the Holmgren-norm of A.

We note that

$$\|A\| \leqslant \|A\|_H .$$

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